

Structural Precursor for the Freezing Transition and Changes of Entropy in Colloids

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The changes in the interactions between particles are important features of colloidal systems. Using classical molecular dynamics simulations, we identify that the changes in the width of the interaction potential of colloidal particles are a trigger of a structural precursor for the freezing transition in the system. Such evidence is manifested as a shoulder just before the second peak of the radial distribution function, in the same manner as it occurs in systems of hard spheres and disks [1]. From the thermodynamic point of view, using a statistical entropy for liquids [2], we evaluate the entropy changes for the nucleation of particles in the precursor stage and the crystallization of the system. The method for the determination of the entropy has been tested with respect to heat capacity experimental data [3] and elsewhere we have also shown that the same formalism can be applied for interacting Brownian particles [4]. In addition in order to survey the approach of the system towards equilibrium, we evaluate the entropy production of the system due to the rearrangement of particles.

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[4] M. Mayorga, L. Romero-Salazar, M. Rubí, Physica A, 307 (2002) 297.